Number of Magic Squares From Parallel Tempering Monte Carlo

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Abstract

There are 880 magic squares of size 4 by 4, and 275,305,224 of size 5 by 5. It seems very difficult if not impossible to count exactly the number of higher order magic squares. We propose a method to estimate these numbers by Monte Carlo simulating magic squares at finite temperature. One is led to perform low temperature simulations of a system with many ground states that are separated by energy barriers. The Parallel Tempering Monte Carlo method turns out to be of great help here. Our estimate for the number of 6 by 6 magic squares is $(0.17745 \pm 0.00016) \times 10^{20}$.

1 Introduction

Magic squares involve using all the numbers $1, 2, 3, ..., n^2$ to fill the squares of an $n \times n$ board so that each row, each column, and both main diagonals sum up to the same number. Interesting information about magic squares is collected at the WEB site of M. Suzuki [1].

We here address the question of the number of magic squares N(n) of a given order n. In the following, this number should always be understood as the total number of magic squares divided by 8, thus considering as equivalent those squares which can be obtained from each other by the obvious reflection and rotation symmetries. It has been known since long that there are 880 magic squares of order 4. N(5) was estimated by L. Candy in his Construction, Classification and Census of Magic Squares of Order Five, privately published in 1938. Candy arrived at a total of 13,288,952. The exact number was determined by Richard Schroeppel in 1973, using a computer backtracking program, see [2]. His result 275,305,224 shows that Candy's estimate was low by a wide margin. It seems very difficult to exactly determine N(n) for n > 5. However, it is possible to obtain statistical estimates with good precision. In this paper we shall describe a Monte Carlo method for this purpose. As a demonstration, we apply it to the cases n=4, 5,and 6. Our method is, however, by no means restricted to theses special cases, and could well be used for higher n, and also for all kinds of variants of magic squares, like pan-magic squares, squares filled with primes only, or magic cubes.

2 Magic Squares at Finite Temperature

We consider magic squares as the zero temperature configurations of a statistical system with partition function

$$Z(\beta) = \sum_{C} \exp[-\beta E(C)], \qquad (1)$$

where the sum is over all possibilities to fill the square with the numbers $n = 1, 2, ..., n^2$. β is proportional to the inverse temperature. We define the energy of a configuration by

$$E(C) = \sum_{\text{columns } c} (S_c - M)^2 + \sum_{\text{rows } r} (S_r - M)^2 + \sum_{\text{diagonals } d} (S_d - M)^2, \quad (2)$$

where S_c , S_r , and S_d are the sums of the columns, rows, and main diagonals, respectively. $M = n(n^2 + 1)/2$ is called the magic constant. Obviously $E(C) \geq 0$. Magic squares have zero energy. The task of counting the number of magic squares N(n) is thus equivalent to counting the number of states of minimal energy, i.e. determining the zero temperature entropy.

Monte Carlo methods allow to estimate expectation values of functions A of the configurations C,

$$\langle A \rangle = \frac{1}{Z} \sum_{C} \exp[-\beta E(C)] A(C).$$
 (3)

Now observe that

$$N(n) = \frac{1}{8} \lim_{\beta \to \infty} Z(\beta). \tag{4}$$

 $Z(\beta)$ is not an expectation value. However, since $Z(0)=(n^2)!,$ we have

$$N(n) = \frac{1}{8} Z(0) \lim_{\beta \to \infty} \langle \exp[-\beta E(C)] \rangle_{\beta=0}, \qquad (5)$$

where the subscript indicates that the expectation value has to be taken at infinite temperature here. Eq. (5) is still not practical for calculations, since for large β the measured quantity $\exp[-\beta E(C)]$ fluctuates over many orders of magnitude, thus leading to very large statistical errors of the Monte Carlo estimate.

Let us therefore consider a collection of β -values $0 = \beta_1 < \beta_2 < \ldots < \beta_m$. Then

$$\frac{Z(\beta_{i+1})}{Z(\beta_i)} = \langle e^{-(\beta_{i+1} - \beta_i)E} \rangle_{\beta_i}, \qquad (6)$$

so that

$$\frac{Z(\beta)}{Z(0)} = \langle e^{-(\beta_2 - \beta_1)E} \rangle_{\beta_1} \langle e^{-(\beta_3 - \beta_2)E} \rangle_{\beta_2} \dots \langle e^{-(\beta_m - \beta_{m-1})E} \rangle_{\beta_{m-1}} \langle e^{-(\beta - \beta_m)E} \rangle_{\beta_m}.$$
(7)

If the β -differences in the measured quantities are not too big, this representations offers a way to compute $Z(\beta)$ for large β and thus an approximation for N(n). We remark that $Z(\beta)$ is strictly monotonously decreasing. The finite β -value therefore yields an upper bound on the number of ground states.

3 Parallel Tempering Monte Carlo

A valid Monte Carlo algorithm to estimate any of the expectation values occurring in eq. (7) can be built using the Metropolis procedure: Propose to exchange the positions of two entries in the square, determine the corresponding energy change ΔE , and implement the modification of configuration with probability

$$p = \min[1, e^{-\beta \Delta E}]. \tag{8}$$

Except for rather small β , the acceptance rates become prohibitively small if one just exchanges randomly selected entries. We therefore restrict the update proposal to the transpositions of 1 with 2, then 2 with 3, ..., $n^2 - 1$ with n^2 . Such moves are also useful in Simulated Annealing procedures designed to search for magic squares with very large n, by minimizing E(C) or a similar cost function.

For larger β -values, naive Monte Carlo simulations run into a problem: The different areas of low energy are separated by high barriers. In order to sample all the low energy contributions with the right weight one has to penetrate and tunnel through these barries. Consequently, very long simulation times are needed.

The situation can be much improved by using the Parallel Tempering or Exchange Monte Carlo method, see, e.g. [3] and further references cited in [4]. It amounts to simulate the joint ensemble of all the (independent) systems with inverse temperatures β_i in parallel. The partition function of this system is

$$Z_{\text{joint}} = \sum_{C_1} \sum_{C_2} \dots \sum_{C_m} \exp[-\beta_1 E(C_1) - \beta_2 E(C_2) - \dots - \beta_m E(C_m)].$$
 (9)

In addition to updating independently the configurations C_i , one includes exchanges of configurations, usually of adjacent β -values. A proposal of such a change is again accepted using a Metropolis procedure. E.g., configurations C_i and C_{i+1} are exchanged with probability

$$p_{i,i+1} = \min[1, e^{-(\beta_{i+1} - \beta_i)(E(C_i) - E(C_{i+1}))}]. \tag{10}$$

The exchange of configurations over the temperature range strongly speeds up the Monte Carlo process at the lower temperatures. Numerical experience shows that, in order for the procedure to be efficient, the acceptance rates for the configuration exchanges should not be very much smaller than one half. Furthermore, having too many systems might also hamper rapid exchange of information from higher to lower temperatures and vice versa.

4 Monte Carlo Results

We simulated squares with n=4, 5 and 6, using always a set of m=20 β -values. The results are summarized in the tables 1, 2, and 3. The largest β -value was chosen such that the acceptance rate $\omega_m = \omega(\beta_m)$ was around one percent. The intermediate β -values were chosen such that the exchange rates in the tempering cycle are roughly of order one half or bigger. Each tempering cycle consisted in performing one Metropolis updating sweep for each of the 20 configurations and then attempting to exchange each of the adjacent β_i -pairs. We made $3.25 \cdot 10^7$ for n=4, and 10^8 such cycles for n=5 and n=6, respectively. This required approximately a total of 12 days on a 166 MHz Pentium PC. The code was not optimized yet with respect to run-time behaviour.

The β_i , the acceptance rates ω_i at β_i , and the exchange rates $\omega_{i,i+1}$ are given in columns 2, 3, and 4 of the tables. The energy expectation value estimates are given in column 5. The last columns of the tables give the ratios of partition functions $Z(\beta_{i+1})/Z(\beta_i)$, where $Z_i = Z(\beta_i)$. The bottom parts present $Z(\beta)/Z(\beta_{20})$ for three extra β -values much larger than β_m . Having three β 's of increasing size allows us to check for convergence of the N(n). The errors of these estimates were obtained by generating 50 synthetic data sets of the Z_{i+1}/Z_i , scattering them around the measured values according to a Gaussian distribution with variances given by the error bars of the simulation results.

Both for n=4 and n=5, our estimates for N(n) stabilize reasonably with increasing β and agree with the exactly known results. Our estimate for N(6) is $0.17745(16) \cdot 10^{20}$.

5 Conclusions

The method proposed provides reliable estimates for the numbers of magic squares. Of course, there remain many possibilities to improve on the simulations (besides going to higher statistics). E.g., one could play around with m, the choices of the β_i and also with the frequency of configuration exchange

attemps.

It would be interesting to complement the present approach with, e.g., analytical methods. High temperature expansions seem feasable. For example, the energy at $\beta = 0$ can be fairly easily evaluated exactly, and is given by $\langle E \rangle_0 = n^2 \, (n^4 - 1)/6$. One can convince oneself that the higher moments of the energy at infinite temperature can all be expressed in closed form, most likely as polynomials in n.

A very short run (10⁶ cycles) for n = 7 yields $N(7) = 0.3760(52) \cdot 10^{35}$. It is an interesting question whether there is some simple behaviour of N(n). Finally, it could be worthwile to study much larger n to look out whether the magic squares at finite temperature have also interesting thermodynamic properties like phase transitions.

References

- [1] http://www.pse.che.tohoku.ac.jp/~msuzuki/MagicSquare.html
- [2] M. Gardner, Scientific American 234 (1976), January, pp. 118 122.
- [3] K. Hukushima, K. Nemoto, cond-mat/9512035.
- [4] E. Marinari, "Optimized Monte Carlo Methods", Lectures given at the 1996 Budapest Summer School on Monte Carlo Methods, condmat/9612010.

n=4 3.25 · 10 ⁷ tempering cycles						
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	β_i	ω_i	$\omega_{i,i+1}$	$\langle E \rangle_{\beta_i}$	Z_{i+1}/Z_i	
1	0.0000	1.000	0.868	680.048(56)	0.520412(29)	
2	0.0010	0.990	0.922	626.364(50)	0.693277(20)	
3	0.0016	0.984	0.861	594.757(51)	0.536070(29)	
4	0.0027	0.973	0.800	539.585(49)	0.427069(34)	
5	0.0044	0.957	0.713	463.419(45)	0.315796(35)	
6	0.0072	0.934	0.631	365.548(32)	0.234237(28)	
7	0.0119	0.902	0.582	262.108(28)	0.196354(33)	
8	0.0195	0.862	0.552	176.937(21)	0.172897(33)	
9	0.0319	0.814	0.529	114.919(11)	0.157632(26)	
10	0.0523	0.754	0.516	72.5736(73)	0.150015(30)	
11	0.0858	0.681	0.508	44.9679(50)	0.148085(27)	
12	0.1407	0.594	0.500	27.3797(28)	0.151383(29)	
13	0.2308	0.491	0.494	16.2867(17)	0.163141(32)	
14	0.3786	0.374	0.495	9.3625(11)	0.188879(35)	
15	0.6208	0.248	0.485	5.08151(74)	0.264513(67)	
16	1.0000	0.118	0.704	2.29517(72)	0.60598(12)	
17	1.3000	0.057	0.813	1.15538(60)	0.78174(11)	
18	1.6000	0.026	0.925	0.55536(40)	0.91600(60)	
19	1.8000	0.015	0.951	0.33992(26)	0.94757(40)	
20	2.0000	0.009		0.20941(20)		
	β			$Z(\beta)/Z_{20}$	$N(\beta)/10^{3}$	
	5.0			0.912727(81)	0.87968(57)	
	8.0			0.912572(81)	0.87953(58)	
	11.0			0.912571(81)	0.87953(58)	
	exact				0.880	

Table 1: Monte Carlo results for n=4.

	n = 5 10 ⁸ tempering cycles					
i	eta_i	ω_i	$\omega_{i,i+1}$	$\langle E \rangle_{\beta_i}$	Z_{i+1}/Z_i	
1	0.0000	1.000	0.561	2600.09(17)	0.10558(15)	
2	0.0010	0.982	0.730	1585.362(97)	0.29389(21)	
3	0.0017	0.971	0.633	1188.134(67)	0.19578(19)	
4	0.0029	0.955	0.551	816.665(45)	0.13749(16)	
5	0.0049	0.934	0.495	527.305(33)	0.10641(13)	
6	0.0084	0.907	0.462	327.343(19)	0.09006(13)	
7	0.0142	0.873	0.442	198.631(11)	0.08139(10)	
8	0.0241	0.831	0.431	118.9178(64)	0.07663(10)	
9	0.0410	0.777	0.424	70.6331(35)	0.07403(10)	
10	0.0698	0.710	0.421	41.7659(21)	0.0726609(97)	
11	0.1186	0.626	0.419	24.6289(12)	0.0719532(95)	
12	0.2016	0.525	0.418	14.48913(70)	0.0716943(94)	
13	0.3427	0.409	0.418	8.50502(44)	0.0718681(90)	
14	0.5826	0.285	0.415	4.90719(32)	0.073181(11)	
15	0.9905	0.165	0.347	4.90719(32)	0.093419(26)	
16	1.6838	0.058	0.810	2.21324(49)	0.659590(71)	
17	1.9000	0.039	0.779	1.65545(52)	0.66774(10)	
18	2.2000	0.021	0.881	1.07235(50)	0.830839(79)	
19	2.4000	0.014	0.903	0.79392(47)	0.871964(76)	
20	2.6000	0.009		0.58657(42)		
	β			$Z(\beta)/Z_{20}$	$N(\beta)/10^9$	
	5.6000			0.66293(25)	0.27914(19)	
	8.6000			0.65469(26)	0.27577(19)	
	11.6000			0.65429(26)	0.27550(19)	
	exact				0.275305204	

Table 2: Monte Carlo results for n = 5.

		n=6	10^8 tempering cycles		
i	eta_i	ω_i	$\omega_{i,i+1}$	$\langle E \rangle_{\beta_i}$	Z_{i+1}/Z_i
1	0.0000	1.000	0.513	7768.23(61)	0.070860(14)
2	0.0004	0.988	0.638	5615.65(36)	0.168908(18)
3	0.0008	0.979	0.502	4352.01(27)	0.086142(13)
4	0.0014	0.966	0.403	2976.04(19)	0.0494970(93)
5	0.0027	0.948	0.345	1827.89(12)	0.0342720(72)
6	0.0052	0.924	0.314	1046.796(62)	0.027587(58)
7	0.0099	0.892	0.298	576.290(33)	0.0244279(51)
8	0.0188	0.849	0.289	310.555(17)	0.0228945(51)
9	0.0358	0.791	0.285	165.4935(79)	0.0221136(43)
10	0.0679	0.713	0.283	87.6788(38)	0.0216969(42)
11	0.1291	0.612	0.282	46.3095(20)	0.0214833(42)
12	0.2452	0.486	0.281	24.4166(11)	0.0213753(44)
13	0.4660	0.340	0.282	12.86353(59)	0.0213645(47)
14	0.8853	0.193	0.235	6.74920(32)	0.0262622(88)
15	1.6821	0.065	0.790	2.91925(39)	0.570565(54)
16	1.9000	0.045	0.824	2.25025(44)	0.672457(64)
17	2.1000	0.031	0.844	1.73410(48)	0.738535(73)
18	2.3000	0.021	0.930	1.31250(49)	0.884956(43)
19	2.4000	0.018	0.877	1.13603(48)	0.821399(76)
20	2.6000	0.012		0.84515(46)	
	β			$Z(\beta)/Z_{20}$	$N(\beta)/10^{20}$
	6.6000			0.55845(25)	0.17842(16)
	10.6000			0.55542(25)	0.17745(16)
	14.6000			0.55536(25)	0.17744(16)

Table 3: Monte Carlo results for n = 6.